

Path Integral Variational Methods for Strongly Correlated Systems

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Abstract

We introduce a new approach to highly correlated systems which generalizes the Fermi Hypernetted Chain and Correlated Basis Function techniques. While the latter approaches can only be applied to systems for which a non-relativistic wave function can be defined, the new approach is based on the variation of a trial hamiltonian within a path integral framework and thus can also be applied to relativistic and field theoretical problems. We derive a diagrammatic scheme for the new approach and show how a particular choice of the trial hamiltonian corresponds exactly to the use of a Jastrow correlated

ansatz for the wave function in the Fermi Hypernetted Chain approach. We show how our new approach can be used to find upper bounds to ground state energies in systems which the FHNC cannot handle, including those described by an energy-dependent effective hamiltonian. We demonstrate our approach by applying it to a quantum field theoretical system of interacting pions and nucleons.

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I. INTRODUCTION

Variational methods provide extremely powerful tools for analyzing complicated many-body hamiltonians. Fermi Hypernetted Chain (FHNC) techniques, in particular, have been successfully applied to many different problems, ranging from nuclear matter to strongly interacting electrons to liquid helium, where strong correlations between particles dominate the system and prohibit the usual perturbative expansions¹⁻³. Correlated Basis Function (CBF) theory, which employs FHNC and cluster summation methods to compute perturbative corrections to quantities determined variationally, has also been successfully applied to a wide variety of systems⁴⁻⁷. These methods, however, have up to now been limited to hamiltonian systems for which a nonrelativistic wave function can be defined. In the present work we build upon a previous letter⁸, developing a framework which goes beyond this limitation. Our particular goal is to find a variational method for studying nuclear systems which include dynamical meson exchange. The methods we shall develop, however, are much more general.

The basic idea of our approach is to adopt a Feynman path integral formulation in euclidean space so as to choose a trial hamiltonian which may be determined variationally. This is less restrictive than the usual FHNC approach, where one chooses a variational wave function. The use of a variational principle in Feynman path integrals is nothing new, as we describe in Sec. 2. The novelty is connecting this principle to the extensive existing FHNC calculations. This is a major goal of the present work. We shall show that the FHNC diagrammatic expansion can be recovered as a particular case of a more general expansion based upon Feynman diagrams. Once this contact is made, one may develop extensions of the highly successful FHNC methods for summing up diagrams to be applied in the more general path integral context, thus opening an aspect of the path integral variational method little explored up to now. Such techniques should have a wide range of applications, including possible improvements upon many existing FHNC calculations, as well as the analysis of systems that the usual FHNC cannot handle, such as those described by effective

(time-dependent) hamiltonians.

The path integral formulation has another advantage: it yields a perturbative expansion which is more compact, as well as more general, than that of time-independent perturbation theory. This can be a great technical advantage — for example, one Feynman diagram with n interaction lines corresponds in principle to $n!$ different Goldstone diagrams. The path integral formulation thus provides a convenient setting for the study of strongly interacting systems: the variational principle can be used to find a trial hamiltonian which reproduces as closely as possible the physics of the true hamiltonian, and the corrections can be calculated within a natural perturbative framework. Since it is usually a matter of some art to choose a trial hamiltonian which successfully balances the competing demands of accuracy and simplicity, a framework which allows a ready interplay between the determination of a variational minimum and perturbative corrections is clearly very useful.

The essential simplification which we shall adopt in choosing a trial hamiltonian is motivated by the FHNC expansion. Whereas a normal perturbative approach builds collective states from independent particles, the FHNC instead treats interparticle correlations as fundamental. Our idea is thus to choose a trial hamiltonian h_0 containing a nontrivial two-body piece which may be varied to reproduce as best as possible the interactions in the true hamiltonian h , but we shall require the one-body part of h_0 to have a highly simplified form with respect to that of h . In contrast to this, the usual perturbative expansion takes h_0 to be just the one-body kinetic energy operator, with no two-body term. Our choice, instead, gives the interactions a more fundamental role; and the simplification of the one-body part shall allow us, as in the FHNC expansion, to sum entire classes of diagrams which give important contributions in strongly correlated systems.

As a matter of fact, we shall choose a one-body piece which depends on a single parameter α , and we shall demonstrate that the choice $\alpha = 0$ (which corresponds to “turning off” the one-body piece completely) exactly reproduces the FHNC expansion. So one immediate result of our formulation is that we can now calculate upper bounds on effective hamiltonians by using the full machinery of the usual FHNC approach. The choice $\alpha = 0$ is essentially a

static approximation, and to go beyond this approximation one must either take $\alpha > 0$ or include higher order corrections in the perturbation $h - h_0$. If we take $\alpha > 0$, we must extend the FHNC techniques for summing diagrams, because now the time integrations are no longer trivial. While it is surely possible to use finite temperature techniques to generalize the FHNC diagrammatic summation so that α may be treated as a true variational parameter, in the present work we shall be content with looking at the particular case $\alpha \rightarrow \infty$. In this limit, the time integrations simplify considerably, and we shall show a particular example of how to sum up diagrams in analogy with the FHNC expansion.

For the particular case $\alpha = 0$, the trial hamiltonian h_0 is directly related to a trial wave function of the CBF type, with the correlations in the CBF wave function corresponding directly to the interactions in h_0 . Of course, as with the CBF correlations, there is a lot of freedom in choosing the two-body part of h_0 . Obviously, the closer one can make this to that of h , the better one's variational estimate of the energy will be. The inclusion of state dependence (that is, spin and isospin dependence) in h_0 clearly improves variational estimates, although in the usual FHNC there are nevertheless many difficulties in implementing this generalization. A popular approximation is the so-called Single Operator Chain approximation², which consists of summing chains of single operator correlations without hyperconnecting them. However, it seems necessary to go beyond the SOC⁹, and it is not yet well understood how to do this. A new approach using spin coherent-state wave functions currently being developed¹⁰ is one possibility. While the present approach may very well provide an alternative means of improvement in this direction, either by allowing for a more complete summation of state-dependent correlations through techniques developed for nonzero α or by allowing for a more straightforward calculation of state-dependent corrections through perturbation theory, we shall limit ourselves in the following to an h_0 which contains only spin-independent two-body interactions. This corresponds to using the the Jastrow (state-independent) correlated trial wave function ansatz. The study of how best to include state-dependent correlations will thus be an important immediate application of the approach we develop here.

The outline of the paper is as follows. We describe the variational principle in the path integral setting and discuss the choice of the trial hamiltonian in Sections 2 and 3. Sections 4 through 6 are concerned with obtaining the usual FHNC diagrammatic scheme as a particular limit of a more general Feynman diagrammatic scheme. In the process of demonstrating this, we show that simplifications which allow the use of FHNC techniques for summing diagrams do not occur in general. In Section 7, in a different limit from that which recovers the FHNC diagrammatic scheme, we show how diagrams may be summed in a different way, and hint at generalizations of the FHNC techniques for this case. In Section 8 we demonstrate our procedure by applying it to a nuclear system containing dynamical pions. Finally, in Section 9 we discuss our results and point toward directions for future study.

II. THE VARIATIONAL PRINCIPLE IN TERMS OF FEYNMAN PATH INTEGRALS

The original idea of formulating the variational principle in the path integral context is due to Feynman himself^{11,12}. Let us briefly summarize here the formalism.

As is well known, the ground state energy of a system can be expressed in terms of the partition function according to

$$E_0 = - \lim_{\beta \rightarrow \infty} \frac{\log Z}{\beta} . \quad (1)$$

On the other hand, the partition function can be expressed in a path integral form as

$$Z = \int D[\psi^\dagger, \psi] e^{-\int_{-\beta/2}^{\beta/2} h[\psi^\dagger, \psi] d\tau} , \quad (2)$$

where we have assumed that the system can be described in terms of a field ψ (either fermionic or bosonic) and its hermitian conjugate. Here $h[\psi^\dagger, \psi]$ is the classical hamiltonian. More precisely, when some ambiguities arise in performing the L egendre transformation, we should start from the lagrangian of the system $L[\psi^\dagger(t), \psi(t)]$ and make the transformation to the euclidean world (imaginary time) $t \rightarrow it = \tau$.

Once a representation of Z is provided, we can define an average over the functional space where the Feynman-Kač integral (2) is defined, namely,

$$\langle f \rangle_{h_0} = \frac{1}{Z_0} \int D[\psi^\dagger, \psi] e^{-\int_{-\beta/2}^{\beta/2} h_0[\psi^\dagger, \psi] d\tau} f[\psi^\dagger, \psi] , \quad (3)$$

with

$$Z_0 = \int D[\psi^\dagger, \psi] e^{-\int_{-\beta/2}^{\beta/2} h_0[\psi^\dagger, \psi] d\tau} . \quad (4)$$

The weight function $e^{-\int_{-\beta/2}^{\beta/2} h_0[\psi^\dagger, \psi] d\tau}$ must be positive definite, which only implies that h_0 must be real. Using this definition the partition function can be rewritten in the form

$$Z = \int D[\psi^\dagger, \psi] e^{-\int_{-\beta/2}^{\beta/2} h_0[\psi^\dagger, \psi] d\tau} \left\langle e^{-\int_{-\beta/2}^{\beta/2} [h - h_0] d\tau} \right\rangle_{h_0} . \quad (5)$$

Now, it is a general property of a mean that

$$\langle e^A \rangle \geq e^{\langle A \rangle} . \quad (6)$$

Thus, applying this last inequality to (5) and inserting into (1), we find

$$E_0 \leq \lim_{\beta \rightarrow \infty} \frac{1}{\beta} \left[-\log \left(\int D[\psi^\dagger, \psi] e^{-\int_{-\beta/2}^{\beta/2} h_0 d\tau} \right) + \left\langle \int_{-\beta/2}^{\beta/2} h d\tau \right\rangle_{h_0} - \left\langle \int_{-\beta/2}^{\beta/2} h_0 d\tau \right\rangle_{h_0} \right] . \quad (7)$$

The first term on the r.h.s. of (7) cancels with the third. This outcome is rather obvious if h_0 is time independent. In this case the first term is by definition the ground state energy of the hamiltonian (being time independent and real, h_0 can in fact be regarded as a hamiltonian) and the third term is the expectation value of the same hamiltonian in the ground state, hence the cancellation. However, since we are interested in extending the variational scheme to effective hamiltonians and therefore want to maintain the possibility of a time dependence in h_0 , we need a more refined proof, which we present in Appendix A. There we show that even for time-dependent potentials, we end up with

$$E_0 \leq \lim_{\beta \rightarrow \infty} \frac{1}{\beta} \left\langle \int_{-\beta/2}^{\beta/2} h(\tau) d\tau \right\rangle_{h_0} . \quad (8)$$

Reexamining the derivation of (8), we see that the functional integral describing Z requires, in order to ensure its existence, that h must be real and bounded from below. A possible dependence upon the time in h (or conversely, in energy-momentum space, upon the energy) cannot be ruled out on the ground of mathematical reasons. We know that the hamiltonian is energy-independent indeed, but it can be useful sometimes to derive an effective hamiltonian, whose energy-dependence is the price we pay for having eliminated some unwanted degrees of freedom. Even in this case the previous procedure applies safely with the only constraint that the effective hamiltonian (obviously bounded from below because the original one is) must be real in the euclidean world (that is, after the replacement $E \rightarrow iE$).

The same consideration applies to h_0 as well, which is nothing but a weight function, even if it will be referred to in the following as a “trial hamiltonian”: again, the only condition h_0 must fulfill for the variational principle (8) to be mathematically well-defined is that it must be real. Of course, for the $\beta \rightarrow \infty$ limit to be physically meaningful, we require that h_0 must have an unique ground state. This is related to the choice of boundary conditions in (2), as we shall see in Sec. 4. For the present we simply note that the inequality is valid independent of the boundary conditions on the path integral, and indeed also for finite β . Thus we have a variational principle

$$F_0 \equiv -\log Z_0 + \left\langle \int_{-\beta/2}^{\beta/2} [h - h_0] d\tau \right\rangle_{h_0} \geq -\log Z \quad (9)$$

for any Z of the form (2), and the boundary conditions and $\beta \rightarrow \infty$ limit must be chosen so as to make F_0 correspond to the quantity in which we are interested, namely, the ground state energy.

Starting from (5), we may also find perturbative corrections in $h_I \equiv h - h_0$ to the variational energy (8) by simply expanding the ratio

$$Z' = \frac{Z}{Z_0} = \left\langle e^{-\int_{-\beta/2}^{\beta/2} h_I d\tau} \right\rangle_{h_0} \quad (10)$$

in Feynman diagrams. Because of the exponentiation property of connected diagrams, we may write immediately

$$\ln Z' = \left\langle e^{-\int_{-\beta/2}^{\beta/2} h_I d\tau} \right\rangle_{h_0}^C = \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} \left\langle \left(\int_{-\beta/2}^{\beta/2} h_I d\tau \right)^n \right\rangle_{h_0}^C, \quad (11)$$

where $\langle \dots \rangle^C$ denotes connected diagrams. The quantity $W \equiv \ln Z = \ln Z_0 + \ln Z'$ is thus the sum of connected Feynman diagrams containing no h_I interaction lines, one h_I line, two h_I lines, and so on. One easily sees that to first order $-\lim_{\beta \rightarrow \infty} W/\beta$ is the variational energy (8), and the higher orders bring in the corrections. There will of course be a delicate interplay between how far one wants to proceed in optimizing the trial hamiltonian h_0 and how far one wants to be able to go in calculating perturbative corrections, decisions which will depend greatly upon the particular system one is studying and upon the particular quantities one is interested in calculating. We see here that the Feynman path integral formulation provides a convenient framework for arriving at such decisions.

III. THE TRIAL HAMILTONIAN

Different choices of h_0 lead to different approximation schemes. For instance, we could choose h_0 in the form of a single-particle kinetic energy operator. It is immediately seen that in such a case the variational method coincides with the first order of the usual perturbative expansion. We could however assume h_0 in the form of a single particle operator but retain a possible time dependence. This topic could give rise to interesting investigations, because very much in the same line Feynman investigated the problem of the polaron, obtaining numerical results far better than the ones provided by the standard techniques (perturbation theory and canonical transformations)¹¹.

The problem can also be handled at a different level, by introducing a more complicated trial hamiltonian having not just a single particle but also a two particle term. The condition we require, of course, is that these hamiltonians can be handled, technically, much more easily than the full hamiltonian of the system. Since a many body system is intrinsically complicated by the presence of the two-body interaction, no matter how simple this interaction is, the possibility we might explore instead is to simplify as far as possible the

single particle term. In this respect two options naturally arise, as we shall discuss in the following.

Consider first a general lagrangian of a system in the real world, namely

$$L = i \int d^3x \dot{\psi}^\dagger(x) \psi(x) - \int d^3x d^3x' \psi^\dagger(x) \epsilon(x, x') \psi(x') - \frac{1}{2} \int d^3x d^3x' \psi^\dagger(x) \psi^\dagger(x') U(|\mathbf{x} - \mathbf{x}'|) \psi(x') \psi(x), \quad (12)$$

where ψ is taken from now on to represent a fermionic field. Here we shall assume the system is translationally invariant, so in 3-momentum space this becomes

$$L = i \sum_q \dot{a}_q^\dagger a_q - \sum_q \epsilon_q a_q^\dagger a_q - \tilde{U} \quad (13)$$

where the a , a^\dagger are the Fourier transforms of the field operators, depending upon time and momentum, and with \tilde{U} we have denoted the Fourier transform of the potential part of the lagrangian; ϵ_q is usually taken to be the single particle kinetic energy. Two obvious simplifications could be to approximate this single particle energy either as zero or as a step function: attractive below the Fermi sea and repulsive above. These two cases are intrinsically different, as we shall see in detail in the following. We can handle them together by setting

$$\epsilon_q \longrightarrow \Delta \theta(q - k_F) - \Delta \theta(k_F - q) ; \quad (14)$$

the former case is obtained from (14) by taking the limit $\Delta \rightarrow 0$.

These two possible choices deserve further comment before proceeding. The former has, as we shall show, the great advantage of being able to reproduce the FHNC diagrammatic scheme. The latter instead will provide the same diagrams although with different coefficients, but nevertheless displays two advantages: namely, it provides a naturally well-defined ground state and furthermore the calculations, when dynamical pions will be introduced, will turn out to be more appropriate. This is because the latter case allows for a more general choice of the two body term \tilde{U} .

For the sake of definiteness we write the lagrangian in the form

$$L = \sum_q \dot{a}_q^\dagger a_q - \Delta \sum_q \theta(q - k_F) a_q^\dagger a_q + \Delta \sum_q \theta(k_F - q) a_q^\dagger a_q - \tilde{U} \quad (15)$$

and its corresponding euclidean version

$$L_E = L(t \rightarrow i\tau) , \quad (16)$$

and then we identify L_E with h_0 . We mention here that the calculations, because of subtleties which we shall detail in the next section, are to be performed at finite β and nonzero Δ and that only at the end of the calculation shall we decide in what order we want to take the limits.

To summarize, the fundamental idea in the present scheme (and the same happens in the FHNC) is that the drastic assumption made on the single particle part of h_0 greatly simplifies the diagrammatic expansion of (8) because all frequency integrations become trivial and the four-dimensional problem reduces to a 3-dimensional one with constant energy denominators.

Finally, we should mention that once we choose an h_0 that is sufficiently complicated — and the presence of a two-body term ensures this — then we are forced to make approximations in evaluating the variational energy E_0 . Of course, an approximation to E_0 need not be an upper bound on the true ground state energy; and thus we need to have a sufficiently robust method for summing diagrams in an expansion in h_0 to allow us to control the approximations made and to ensure that the calculated energies converge systematically toward the true variational energy E_0 . The FHNC scheme has been successful in this respect, at least in the case of spin-independent correlations, and so we model our approach upon that scheme.

IV. CONNECTION WITH THE FHNC EXPANSION

The average value of a local, two-body potential V taken over a Jastrow correlated wave function can be written as

$$\langle \psi_J | V | \psi_J \rangle = \langle \phi_0 | e^{\mathcal{U}/2} V e^{\mathcal{U}/2} | \phi_0 \rangle \quad (17)$$

where $|\psi_J\rangle$ is the Jastrow-correlated approximation to the ground state, whose wave function is

$$\psi_J(r_1, \dots, r_N) = \hat{G}\phi_0(r_1, \dots, r_N) . \quad (18)$$

Here $\hat{G} = e^{\mathcal{U}/2}$ is the Jastrow correlation operator

$$\hat{G} = \prod_{ij} f(r_{ij}) , \quad (19)$$

$|\phi_0\rangle$ is the Free Fermi Gas ground state, and $\phi_0(r_1, \dots, r_N)$ is the corresponding Slater determinant wave function.

We wish to show that the same result comes out from the formula

$$\begin{aligned} \langle V \rangle &= \lim_{\beta \rightarrow \infty} \frac{1}{\beta} \int D[\psi^\dagger, \psi] \\ &\int d^4x d^4y V(x-y) \psi^\dagger(x) \psi^\dagger(y) \psi(y) \psi(x) e^{-\int_{-\beta/2}^{\beta/2} d\tau L_E(\tau)} \end{aligned} \quad (20)$$

where $V(x-y) = V(|\mathbf{x} - \mathbf{y}|)\delta(x_0 - y_0)$, provided a suitable connection between \mathcal{U} and \tilde{U} is found. At first sight the connection is simple. Since V is time independent, we can replace (20) with

$$\begin{aligned} \langle V \rangle &= \lim_{\beta \rightarrow \infty} \int D[\psi^\dagger, \psi] \int d^3x d^3y V(|\mathbf{x} - \mathbf{y}|) \\ &\psi^\dagger(\mathbf{x}, 0) \psi^\dagger(\mathbf{y}, 0) \psi(\mathbf{y}, 0) \psi(\mathbf{x}, 0) e^{-\int_{-\beta/2}^{\beta/2} d\tau L_E(\tau)} , \end{aligned} \quad (21)$$

which can be rewritten, using the definition of the path integral, as

$$\langle \phi_0 | \mathcal{T} \left(V(0) e^{-\int_{-\beta/2}^{\beta/2} L_E d\tau} \right) | \phi_0 \rangle = \langle \phi_0 | e^{-\int_0^{\beta/2} L_E d\tau} V e^{-\int_{-\beta/2}^0 L_E d\tau} | \phi_0 \rangle \quad (22)$$

and, since U is also time independent, (22) coincides with (17) if we take $L_E = -\mathcal{U}/\beta$, that is,

$$U = -\frac{1}{\beta} \mathcal{U} \quad \text{and} \quad \Delta = 0 . \quad (23)$$

Note that we have not invoked any commutation properties between U and V , and thus the expressions (17) and (20) are also equivalent if we replace V by the kinetic energy T . These

are in fact particular instances of a more general equivalence. For example, we could replace V in these equations by a nonlocal two-body operator

$$\mathcal{O} = \sum_{kpk'p'} O_{kpk'p'} a_k^\dagger a_p^\dagger a_{p'} a_{k'}, \quad (24)$$

and the expressions would still be equivalent. This implies, by means of functional derivation with respect to O , that the two-body density matrices derived from (17) and (20) also coincide. It follows that the averages of the kinetic energy from the Jastrow ansatz and from the path integral approach also coincide. We limit our discussion here to a local, two-body operator for simplicity.

In writing down (22) we have chosen a particular set of boundary conditions for our path integral. This shall be discussed presently, but it is worthwhile here to first remind the reader of our goal. The point is that (20) is much more general than (17); in particular, there is no need to restrict the potentials V or U in (20) to be independent of time, whereas this is necessary if we use V and \mathcal{U} in (17) (just as we call $h_0 = L_E$ the trial hamiltonian, we shall generally refer to the correlations U and \mathcal{U} as potentials). Thus our ultimate goal is to develop a diagrammatic scheme for calculating (20). Here we are concerned with showing that in the particular case when we choose a V and a U that can be handled by the FHNC scheme arising from (17), then for the choice (23) our new diagrammatic scheme will give exactly that of the FHNC.

It is natural in this respect, starting from (20), to introduce a perturbation expansion in U . First we define the generating functional in the presence of external sources

$$Z[\eta, \eta^\dagger] = \int D[\psi^\dagger, \psi] e^{i \int_{-\beta/2}^{\beta/2} [L(t) + \psi^\dagger(t) \eta(t) + \eta^\dagger(t) \psi(t)] dt} \quad (25)$$

and its euclidean counterpart:

$$Z_E[\eta, \eta^\dagger] = Z[\eta, \eta^\dagger] \Big|_{t \rightarrow i\tau}, \quad (26)$$

so that the average of the potential V reads

$$\langle V \rangle = \quad (27)$$

$$\int d^4x d^4y V(x-y) \frac{\delta}{\delta\eta(x)} \frac{\delta}{\delta\eta(y)} \frac{\delta}{\delta\eta^\dagger(y)} \frac{\delta}{\delta\eta^\dagger(x)} Z_E[\eta, \eta^\dagger] \Big|_{\eta, \eta^\dagger=0} .$$

Note that whether one uses a quantum-mechanical (real time) or a statistical (imaginary time) approach is irrelevant in determining a static quantity (a real number) like the average of V . Thus we can use indifferently the generating functional or the partition function in the following, at least as long as we are interested in static (ground state) properties of the system. The study of linear responses should instead be dealt with only in the quantum-mechanical frame.

The perturbation expansion is now carried out on the generating functional by means of the relation

$$Z[\eta, \eta^\dagger] = e^{-i \int d^4x d^4y U(x-y) \frac{\delta}{\delta\eta(x)} \frac{\delta}{\delta\eta(y)} \frac{\delta}{\delta\eta^\dagger(y)} \frac{\delta}{\delta\eta^\dagger(x)}} Z_0[\eta, \eta^\dagger] \quad (28)$$

where $U(x-y) = U(|\mathbf{x} - \mathbf{y}|)\delta(x_0 - y_0)$, the “unperturbed” lagrangian is $L_0 = L + \tilde{U}$, with L given in (15), and

$$Z_0[\eta, \eta^\dagger] = \int D[\psi^\dagger, \psi] e^{i \int_{-\beta/2}^{\beta/2} [L_0(t) + \psi^\dagger(t)\eta(t) + \eta^\dagger(t)\psi(t)] dt} . \quad (29)$$

The reason we have repeated here these straightforward manipulations is that they point out two subtleties of the procedure.

The first subtlety is that the boundary conditions are exploited in explicitly evaluating the path integral in (29), that is, in defining the inverse of the lagrangian L_0 . This free propagator in momentum space reads

$$\mathcal{G}_\Delta^0(\omega_n, q; \beta) = \frac{\theta(q - k_F)}{\omega_n - \Delta + i\eta} + \frac{\theta(k_F - q)}{\omega_n + \Delta - i\eta} \quad (30)$$

with discrete frequencies because the time integration is limited:

$$\omega_n = \frac{n\pi}{\beta} . \quad (31)$$

Here we wish to choose antiperiodic boundary conditions in order that the path integral is equivalent to a trace over fermionic states, and so n is restricted to be an odd integer.

The second subtlety, strictly related to the first, concerns the degeneracy of the unperturbed ground state: as long as Δ is kept finite a unique ground state exists and coincides with the Fermi sphere, and the definition (30) makes sense both for finite β and in the limit $\beta \rightarrow \infty$. Then a perturbation theory can be performed by means of eq. (28). If we put instead $\Delta = 0$ from the very beginning, any independent particle state is degenerate with respect to L_0 and fixing the ground state becomes arbitrary. Thus, taking the limit $\beta \rightarrow \infty$ for $\Delta \neq 0$ picks out the ground state when the boundary conditions on the path integral are chosen as above, that is, so that (29) gives a trace over states. For $\Delta = 0$, however, we must fix the ground state “by hand” — that is, as is detailed in Appendix B, we must choose a more involved set of boundary conditions which explicitly give the states ϕ_0 at $t = -\beta/2$ and ϕ_0^\dagger at $t = \beta/2$ in (28). Moreover, with $\Delta = 0$ the momentum space propagator (30) is then singular in the $\beta \rightarrow \infty$ limit.

To demonstrate that we are truly evaluating the average of V as given in (17) we need the expression of the propagator in configuration space, namely:

$$\begin{aligned} \mathcal{G}_\Delta^0(x, y; \beta) &= \langle \phi_0 | \mathcal{T} \left(\psi(x) \psi^\dagger(y) \right) | \phi_0 \rangle \\ &= e^{-i\Delta|x_0-y_0|} \int \frac{d^3k}{(2\pi)^3} e^{i\mathbf{k} \cdot (\mathbf{x}-\mathbf{y})} \\ &\quad [\theta(x_0 - y_0) \theta(k - k_F) - \theta(y_0 - x_0) \theta(k_F - k)] . \end{aligned} \quad (32)$$

This corresponds to the second choice of boundary conditions discussed above, so that we can properly take the $\Delta \rightarrow 0$ limit. Thus the Fourier transform of (32) is equal to (30) only in the $\beta \rightarrow \infty$ limit (which must be taken in the end, in any case).

With some elementary manipulations and defining the matrix element of the free density matrix in configuration space as

$$\rho(k_F | \mathbf{x} - \mathbf{y}) = \langle \mathbf{x} | \rho | \mathbf{y} \rangle = \int \frac{d^3k}{(2\pi)^3} e^{i\mathbf{k} \cdot (\mathbf{x}-\mathbf{y})} \theta(k_F - |\mathbf{k}|) , \quad (33)$$

we can rewrite (32) in the form

$$\mathcal{G}_\Delta^0(x, y; \beta) = e^{-i\Delta|x_0-y_0|} \{ \theta(x_0 - y_0) \delta(\mathbf{x} - \mathbf{y}) - \rho(k_F | \mathbf{x} - \mathbf{y}) \} . \quad (34)$$

In the euclidean world, one has

$$\mathcal{G}_{\Delta E}^0(x, y; \beta) = e^{-\Delta|x_0-y_0|} \{ \theta(x_0 - y_0) \delta(\mathbf{x} - \mathbf{y}) - \rho(k_F |\mathbf{x} - \mathbf{y}|) \} . \quad (35)$$

To complete the proof that this perturbative expansion leads to the FHNC diagrams it is now sufficient to follow the derivation of the FHNC diagrams given in¹³: there it is shown that the FHNC diagrams are obtained from a Feynman diagram expansion followed by time integration (we shall show this in some detail in Sec. 6). The identification (23) provides the link between the potentials, and the free Green's function is nothing but $\mathcal{G}_{\Delta E}^0(x, y; \beta) |_{\Delta=0}$.

Thus we can conclude that the FHNC diagrammatic scheme exactly follows from the perturbation expansion (28) in the limit $\Delta \rightarrow 0$ followed by the limit $\beta \rightarrow \infty$. We stress that it need not be equivalent — and this is indeed the case — if one exchanges the order of these limits. We can infer the reason for this trouble. It is apparent in fact from (35) that two cutoffs are present, the first being β and the second Δ , and dropping the first or the second need not necessarily give the same results. It will be proved in the next section that the two expansions obtained by taking the limits in different orders are in fact not equivalent.

V. THE ORDER OF THE LIMITS $\beta \rightarrow \infty$ AND $\Delta \rightarrow 0$

The fundamental task in constructing the FHNC diagrams is to perform, in some way, the time integrations in the Feynman diagrams, in order to get a static or 3-dimensional theory. As a first step we prove, as a byproduct, that the two limits we discussed before are indeed not equivalent. We consider for simplicity in this section only vacuum to vacuum diagrams, but of course the procedure can be easily generalized to any kind of Green's function.

To start with, let us consider a generic Feynman diagram of order n (that is, a diagram that contains n potential lines). It will contain, of course, $2n$ fermionic lines \mathcal{G}_{Δ}^0 , which we write in the form (32), in which the different time orderings are explicit. We shall work in

configuration space, and we are now interested in carrying out the time integrations. The general form of the diagram will be

$$\frac{1}{\beta} \int d^3x_1 \dots d^3x_n \int_{-\frac{\beta}{2}}^{\frac{\beta}{2}} d\tau_1 \dots \int_{-\frac{\beta}{2}}^{\frac{\beta}{2}} d\tau_n \prod \mathcal{G}_{\Delta}^0(x_i, x_j; \beta) \prod U(|\mathbf{x}_k - \mathbf{x}_l|), \quad (36)$$

where we have divided by β in order to take the $\beta \rightarrow \infty$ limit.

As a first step we can break the time integration region in $n!$ parts, each one characterized by a definite ordering of the times. For a given ordering in eq. (36), then, only one of the two terms composing the Green's function (32) can contribute. So each line is characterized by its propagation forward or backward in time, and the $n!$ terms so obtained are, in general, different — although, in practice, many are equivalent. We will refer to them — improperly — as Goldstone diagrams. We observe that all Goldstone diagrams derived from the same Feynman diagram have the same spatial part, and it is only the time integrations which are, in principle, different.

Having chosen a Feynman diagram and having expanded it in Goldstone diagrams, let us further select one of these diagrams and perform its time integrals. The diagram is characterized by n time variables, in a given time ordering. Let them be $\tau_1 < \tau_2 < \dots < \tau_n$. The θ -functions will then be absorbed into the integration limits. The time attenuation factors $e^{-\Delta|\tau_i - \tau_j|}$ remain, but now all absolute values can be removed. It can be easily seen that in any diagram, for each potential line taken at a time τ , each propagator connected to the potential line from below (no matter if incoming or outgoing) carries a factor $e^{-\Delta\tau}$ and each propagator connected from above carries a factor $e^{\Delta\tau}$. Now let us make a trick. For each fermion line crossing but not stopping at a given time τ_i let us insert the factors $e^{\Delta\tau_i} e^{-\Delta\tau_i}$. Then let us collect together all the factors $e^{-\Delta(\tau_{i+1} - \tau_i)}$. Their number is just the number of fermion lines flowing between τ_i and τ_{i+1} (including, then, also those which do not end at τ_i or τ_{i+1}). Thus let us call n_1 the number of fermion lines flowing between τ_1 and τ_2 and, more generally, n_i those between τ_i and τ_{i+1} . The time part of the diagram will then be

$$I(\beta, \Delta) = \frac{1}{\beta} \int_{-\frac{\beta}{2}}^{\frac{\beta}{2}} d\tau_n \int_{-\frac{\beta}{2}}^{\tau_n} d\tau_{n-1} \dots \int_{-\frac{\beta}{2}}^{\tau_3} d\tau_2 \int_{-\frac{\beta}{2}}^{\tau_2} d\tau_1 \prod_{i=1}^{n-1} e^{-n_i \Delta (\tau_{i+1} - \tau_i)} . \quad (37)$$

Now consider the two different limits:

1. $\Delta \rightarrow 0$

In this case the integral is trivial: we get

$$I(\beta, \Delta) = \frac{\beta^{n-1}}{n!} . \quad (38)$$

2. $\beta \rightarrow \infty$

Changing variables to $\lambda_i = \tau_i - \tau_{i+1}$ and $\tau_n \rightarrow \beta \tau_n$, we find

$$\lim_{\beta \rightarrow \infty} I(\beta, \Delta) = \int_{-1/2}^{1/2} d\tau_n \int_{-\infty}^0 d\lambda_{n-1} \dots \int_{-\infty}^0 d\lambda_1 \prod_{i=1}^{n-1} e^{n_i \Delta \lambda_i} = \prod_{i=1}^{n-1} \frac{1}{n_i \Delta} . \quad (39)$$

We are now ready to prove the inequivalence of the two limits.

Consider first the diagram of fig. 1: it generates 6 Goldstone diagrams, all equal and all having the same graphical representation as in fig. 1. The time integrations are immediate according to our preceding rules and, accounting for the multiplicity of the diagram, they provide a factor β^2 for the limit $\Delta \rightarrow 0$ and $\frac{6}{16\Delta^2}$ for the limit $\beta \rightarrow \infty$.

Next consider the diagram of fig. 2. It generates 24 Goldstone diagrams: this time, however, not all are equivalent. As a matter of fact, three kinds of diagrams arise, each with multiplicity 8, as shown in fig. 3. Their evaluation is now simple according to our rules. For the sum, we find β^3 in the limit $\Delta \rightarrow 0$, of course, and

$$8 \frac{1}{(4\Delta)^3} + 8 \frac{1}{(4\Delta)^3} + 8 \frac{1}{(4\Delta)^2(8\Delta)} = \frac{5}{16\Delta^3}$$

for the limit $\beta \rightarrow \infty$. It is thus clear that no linear relationship between Δ and β can be found which is able to provide the same result for the two graphs. This counterexample proves the inequivalence between the different orderings of the two limits.

In fact, it is clear from (36) that by re-scaling $U \rightarrow U/\beta$, the time integrations give a factor $\tilde{I}(\alpha) \equiv I(\beta, \Delta)/\beta^{n-1}$, that is, a function of just the product $\alpha \equiv \beta\Delta$. Thus we could send $\beta \rightarrow \infty$ and $\Delta \rightarrow 0$ in such a way that α is finite, and then treat α as a new variational parameter. One can see from (37) that the time integrations are then in general nontrivial. Of course, the results (38) and (39) correspond to $\alpha \rightarrow 0$ and $\alpha \rightarrow \infty$, respectively; and, because the time integrations simplify greatly in these limits, these are the only cases we shall consider in the following.

VI. DERIVATION OF THE FHNC DIAGRAMS

To carry out the time integrations and to derive the FHNC diagrams we start from the separation (34). It is convenient to introduce new symbols in the diagrams. Thus let us set

$$\mathcal{K}_{\Delta}^0(x; \beta) = e^{-i\Delta|x_0|}\theta(x_0)\delta(x) , \quad (40)$$

graphically denoted from now on with a double solid line, and

$$g_{\Delta}^0(x; \beta) = -e^{-i\Delta|x_0|}\rho(k_F|\mathbf{x}|) , \quad (41)$$

denoted by a single line, so that $\mathcal{G}_{\Delta}^0 = \mathcal{K}_{\Delta}^0 + g_{\Delta}^0$. The procedure we shall follow is now, from a given Feynman diagram, to expand it into products of \mathcal{K}_{Δ}^0 and g_{Δ}^0 , thus generating a certain number of new diagrams — which we shall call “intermediate diagrams” — with single and double lines, as exemplified in fig. 4. Then we shall re-sum classes of these new diagrams in order to simplify the subsequent time integrations. In fact, for the case $\Delta = 0$, we can sum together the intermediate diagrams in such a way as to eliminate all time dependence in the fermion lines, so that the time integrations are trivial and the resulting diagrams are equivalent to those of the FHNC expansion.

In order to reproduce the FHNC, of course, we consider potentials U (corresponding to Jastrow correlations) which are independent of time. Thus the only time dependence in the diagrams we are considering comes from the fermion propagators. (For the case $\Delta=0$, in

particular, we see from (40) and (41) that the only time dependence is in the double line propagators \mathcal{K}_Δ^0 .) Thus, if we can demonstrate that we can sum up intermediate diagrams in such a way that — without ever performing any integrations — time dependence can be eliminated in an arbitrary line of fermion propagators, then we will have succeeded in demonstrating that *all* the intermediate diagrams can be summed to form a new set of diagrams which are entirely time independent. Again, for the case $\Delta = 0$, it is in fact sufficient to consider a fermion line consisting of an arbitrary number of double-line propagators preceded and followed by a single line propagator. We shall begin with the simplest case.

To get rid of the time dependence of the intermediate diagrams, we want to cancel the θ -functions carried by the double lines. To this purpose consider first a double line in a generic diagram preceded and followed by a single line, as in fig. 5a. Then another diagram differing from the first only in the subdiagram of fig. 5b surely also exists, independent of what is contained in the rest of the diagram. The subdiagrams plotted in fig. 5 may be summed immediately to provide (in Euclidean space, and with the obvious notational shortcuts $\rho_{ij} = \rho(k_F|\mathbf{x}_i - \mathbf{x}_j|) = \rho_{ji}$ and $\delta_{ij} = \delta(|x_i - x_j|)$)

$$\begin{aligned} \delta_{12}\rho_{13}\rho_{14}e^{-\Delta|t_1-t_2|}\Big[e^{-\Delta|t_1-t_3|}e^{-\Delta|t_2-t_4|}\theta(t_2-t_1) \\ +e^{-\Delta|t_2-t_3|}e^{-\Delta|t_1-t_4|}\theta(t_1-t_2)\Big]. \end{aligned} \quad (42)$$

Two points in this equation deserve comment: first, the spatial part of the diagram is factorized, owing to the spatial δ -function contained in the double line propagator and, second, the time structure is complicated and depends explicitly upon the time ordering, as one can easily verify. It clearly simplifies drastically in the limit $\Delta \rightarrow 0$, however, when it becomes just $\delta_{12}\rho_{13}\rho_{14}$. In this limit, then, the sum of the subdiagrams in fig. 5 is a new, time-independent subdiagram whose spatial part is identical to that of these two subdiagrams.

The next step is to consider the subdiagrams of fig. 6. It is easily realized here that, always in the limit $\Delta \rightarrow 0$, again all the spatial parts factor out and the time part becomes

a sum of θ -functions, just the sum of all possible time orderings, and it gives exactly 1.

The procedure can be iterated in this way for any number of subsequent double lines.

Other particular cases are straightforward. For instance, if the two external lines join at the same point (i.e., $t_3 = t_4$) clearly nothing changes, and the proof follows the same path if the external lines are replaced by a single external line closing the loop (it is sufficient to multiply the diagram by $[g_\Delta^0]^{-1}(x_4 - x_3)$ and to integrate over t_3 and t_4). Since any closed loop must contain at least one single line (because only the single line pieces carry an advanced part) we have proved that, collecting a suitable class of Feynman diagrams together, in any closed loop the θ -functions of \mathcal{K}_Δ^0 cancel out. Since now any closed diagram contains closed loops only, our proof holds true for all closed diagrams. In this case all time dependence disappears, and the time integrations are trivial, giving a factor β^n . Note that this proof does not depend upon the particular form of the dashed (potential) lines. They represent, in general, the two-body part of the trial hamiltonian h_0 , namely $U = -\mathcal{U}/\beta$ (the factors $\frac{1}{\beta}$ cancel the β 's coming from the time integrations), but any one line in a given diagram should be replaced by V , namely, the true potential of the system. In this way the closed diagrams just represent the average value of V in terms of time-independent diagrams.

Before concluding the discussion of the diagrammatic scheme in the limit $\Delta \rightarrow 0$, we want to stress a last detail. It is not always straightforward to determine which diagrams must be collected together in order that the θ -functions sum to 1. The needed diagrams surely exist, *but they could also coincide*. That is, a given symmetry could mean that $n!$ of the necessary diagrams might not correspond to distinct Feynman diagrams. In this case we simply get a factor $1/n!$ in front of the diagram. This is in particular the case for the ladder diagrams of fig. 7. There, clearly, accounting for the factor $1/n!$ and for the locality of the propagators \mathcal{K}_Δ^0 , the sum reads

$$\mathcal{U}(|\mathbf{x} - \mathbf{y}|) + \frac{1}{2}\mathcal{U}^2(|\mathbf{x} - \mathbf{y}|) + \frac{1}{3!}\mathcal{U}^3(|\mathbf{x} - \mathbf{y}|) + \dots = e^{\mathcal{U}} - 1. \quad (43)$$

This provides the still unspecified link between $U = -\frac{1}{\beta}\mathcal{U}$ and the variational parameter $f(r_{ij})$ used in the FHNC. There, in fact, no ladder diagrams are present, but those of fig. 7

can be summed up to give the result (43), so that the desired link is

$$f^2 - 1 = e^{\mathcal{U}} - 1 . \quad (44)$$

Having thus summed together the various classes of intermediate diagrams to obtain a new set of time-independent diagrams, we may shrink the double-line propagators — which now just represent spatial δ -functions — to points. We may furthermore replace each potential line with the ladder sum $e^{\mathcal{U}} - 1$ above. Although more than one potential line can meet at a single point, we must now specify that any two given points can be connected by at most only one potential line so as to avoid overcounting. There is one spatial propagator ρ_{ij} entering and one leaving each point (including the possibility ρ_{ii}), and all diagrams contain only closed fermion loops. This completes the derivation of the FHNC diagrammatic scheme.

Let us now make the following observations. First, it is clear that for $\Delta \neq 0$ our re-summing of intermediate diagrams does not eliminate all time dependence, and we will need to look for a modification of FHNC techniques in order to handle the nontrivial time integrations in this case. Second, we should like to stress once again that our derivation of the FHNC diagrams in the case $\Delta = 0$ is entirely independent of the form of the potentials. In particular, the unlabelled ends of the potential lines in figs. 5 and 6 could be fixed at different times without disrupting the conclusions that the fermion lines in the re-summed intermediate diagrams are time independent. Thus our approach allows for the possibility that the true potential V and/or the correlations U can be time dependent. Because the fermion lines are nevertheless time independent in this latter case, the time integrations of an n th order diagram become simply independent averages of the n potentials over time. Consequently, for the case $\Delta = 0$, there will be no gain in allowing the correlations to depend on time; nevertheless, our formalism now allows us to find variational upper bounds on the ground state energies of time-dependent effective hamiltonians, and no changes in the FHNC machinery are needed to implement this extension. We shall see a specific example of this latter case in sec. 8.

VII. THE DIAGRAMS FOR FINITE Δ

Consider now the case of the limit $\beta \rightarrow \infty$ followed by $\Delta \rightarrow 0$. This time let us make the rescaling $U \rightarrow \Delta U$ and consider any diagram of order U^{N-1} in the expansion of the average of V . After the frequency integrations in momentum space, it is easy to see that there will be $N - 1$ energy denominators which are just multiples of Δ (this can also be seen from our configuration space analysis in sec. 4). Since the diagram also carries $N - 1$ U lines, after the rescaling all the Δ 's cancel so that the result is independent of Δ . Thus the limit $\Delta \rightarrow 0$ is unnecessary. This is, in fact, just a re-statement of our conclusion from sec. 5: namely, that it is only the product $\alpha = \Delta\beta$ which is important here. The FHNC diagrammology is reproduced by taking the $\alpha \rightarrow 0$ limit, and the present case corresponds to the limit $\alpha \rightarrow \infty$.

Apart from the different rescaling, the derivation of the diagrams follows precisely the same steps as in the previous section but, having separated the \mathcal{K}_Δ^0 and the g_Δ^0 lines, the frequency integration provides, as seen before, different coefficients. Once these have been found by explicit integration, then all \mathcal{K}_Δ^0 lines disappear and, up to the different coefficients, we are left with exactly the same diagrams as before. This time, however, the re-summation of the class of diagrams of fig. 7 follows a different path. Let us work in momentum space and let us define $\tilde{U}(q)$ as the Fourier transformed potential and $\tilde{\Gamma}(p, k; q)$ as the sum of the ladder diagrams, p and k being the momenta entering the diagrams. Clearly $\tilde{\Gamma}(p, k; q)$ fulfills the Bethe-Salpeter equation

$$\begin{aligned}\tilde{\Gamma}(p, k; q) &= \tilde{U}(q) + i \int \frac{d^4 t}{(2\pi)^4} \frac{\tilde{\Gamma}(p, k; t) \tilde{U}(q - t)}{(p_0 + t_0 - \Delta + i\eta)(k_0 - t_0 - \Delta + i\eta)} \\ &= \tilde{U}(q) + \frac{1}{k_0 + p_0 - 2\Delta + i\eta} \int \frac{d^3 t}{(2\pi)^3} \tilde{\Gamma}(p, k; t) \tilde{U}(q - t) .\end{aligned}\tag{45}$$

Going to configuration space, this equation is immediately solved. Calling x_1 , x_2 and $y_1 - y_2$ the transforms of p , k and q , we get

$$\Gamma(x_1^0, x_2^0, y_1 - y_2) = \int_{-\infty}^{\infty} \frac{dp_0}{2\pi} \int_{-\infty}^{\infty} \frac{dk_0}{2\pi} e^{ip_0(x_1^0 - y_1^0) + ik_0(x_2^0 - y_2^0)}\tag{46}$$

$$\frac{U(\mathbf{y}_1 - \mathbf{y}_2)}{1 - \frac{U(\mathbf{y}_1 - \mathbf{y}_2)}{k_0 + p_0 - 2\Delta + i\eta}} \delta(y_1^0 - y_2^0)$$

which still depends upon the initial times.

However, we recall that *no conditions have been imposed upon the possible time (or energy) dependence of U* . In particular, we can rewrite the trial hamiltonian (now, strictly, no longer a hamiltonian) as

$$h_0 = \sum_{k > k_F} \Delta a_k^\dagger a_k - \sum_{k < k_F} \Delta a_k^\dagger a_k + \Delta \sum_{kpq} \tilde{\lambda}(k, p; \mathbf{q}) a_p^\dagger a_k^\dagger a_{k-q} a_{p+q} \quad (47)$$

where we explicitly allow an energy dependence in the “effective potential” $\tilde{\lambda}$ upon the initial energies k_0 and p_0 but not upon the transferred energy q_0 . We can now write down the Bethe-Salpeter equation exactly as before, getting a similar result. Going again to configuration space and calling λ the Fourier transform of $\tilde{\lambda}$ with respect to the spatial coordinates only, we get

$$\Gamma(x_1, x_2, y_1, y_2) = \int_{-\infty}^{\infty} \frac{dp_0}{2\pi} \int_{-\infty}^{\infty} \frac{dk_0}{2\pi} e^{ip_0(x_1^0 - y_1^0) + ik_0(x_2^0 - y_2^0)} \quad (48)$$

$$\frac{\lambda(p_0, k_0, \mathbf{y}_1 - \mathbf{y}_2)}{1 - \frac{\lambda(p_0, k_0, \mathbf{y}_1 - \mathbf{y}_2)}{k_0 + p_0 - 2\Delta + i\eta}} \delta(y_1^0 - y_2^0) .$$

Now we can use the extra energy dependence of λ to remove that of Γ . We can define, in fact,

$$\lambda(p_0, k_0, \mathbf{y}) = \frac{(p_0 + k_0 - 2\Delta) \gamma(\mathbf{y})}{p_0 + k_0 - 2\Delta + \gamma(\mathbf{y})} \quad (49)$$

so that inserting (49) into (47) we get the straightforward result

$$\Gamma(x_1, x_2, y_1, y_2) = \gamma(\mathbf{y}_1 - \mathbf{y}_2) \delta(x_1^0 - y_1^0) \delta(x_2^0 - y_2^0) \delta(y_1^0 - y_2^0) . \quad (50)$$

Thus, having chosen a particular frequency dependence of the effective potential $\tilde{\lambda}$, we can substitute everywhere the potential with the sum of the ladder series Γ , which is now fully

frequency independent. Of course at this stage the only relevant point is the existence of the starting quantity $\tilde{\lambda}$, not its cumbersome form. Naturally, the contact with the FHNC diagrammatic scheme is now provided by $f^2 - 1 = \gamma$.

However, we must remind the reader that in the $\beta \rightarrow \infty$ limit in which we are working now, the coefficients of our diagrams resulting from frequency (or time) integration are not those of the FHNC because the fermion lines are not time independent. We still have to make the connection with FHNC techniques for summing diagrams in this case, for the different coefficients prevent us from summing diagrams through the usual FHNC integral equations. While we shall not pursue this topic further in the present work, we will mention that this $\Delta \neq 0$ case might be handled by extending the FHNC equations to include time integrals, thereby generating the different coefficients as one builds chains and hyperchains. It is convenient to work in configuration space, but to transform from time to frequency variables. Then one arrives at a diagrammatic scheme which is identical to that of the FHNC except that exchange and dynamical correlation lines carry frequency variables, and the points — while still representing spatial δ -functions — now have a nontrivial frequency dependence. Because of the simple form of the single particle term in L_0 , however, one can still classify diagrammatic types in a way similar to that done in the FHNC, forming chains by performing convolution integrals over frequency as well as spatial variables, and forming hyperchains by summing over ladder diagrams as demonstrated here for the simplest type of two-point correlation. An important extension here would be to allow for correlations $\tilde{\lambda}$ in (47) which also depend on the frequency q_0 .

VIII. THE PION EXCHANGE POTENTIAL

Finally we come to a quantum field theoretical model in order to see how it can be embedded in the previous formalism. Consider for the sake of simplicity a system of non-relativistic nucleons interacting with a pionic field through the typical interaction lagrangian

$$L_I = -i \frac{f_{\pi NN}}{m_\pi} \int d^3x \psi^\dagger(x) \left(\boldsymbol{\sigma} \cdot \boldsymbol{\nabla} \vec{\tau} \cdot \vec{\phi}(x) \right) \psi(x) . \quad (51)$$

If L_N and L_π are the free lagrangians for nucleons and pions, respectively, the partition function of the system reads

$$Z = \int D[\psi^\dagger \psi \phi] e^{-\int_{-\beta/2}^{\beta/2} d\tau \{L_N + L_\pi + L_I\}_{t \rightarrow i\tau}} \quad (52)$$

where it must be stressed — and this is the main drawback of the present model — that the term $\lambda\phi^4$ in the lagrangian has been neglected, whereas we know that it is necessarily present in a renormalizable theory. This simplification ensures, however, that the remaining lagrangian is quadratic in the pion field, which can consequently be integrated out. Calculations are straightforward¹⁴ and provide (apart from an inessential constant factor)

$$Z = \int D[\psi^\dagger \psi] e^{-\int_{-\beta/2}^{\beta/2} dx^0 L_N - \int_{-\beta/2}^{\beta/2} dx^0 \int_{-\beta/2}^{\beta/2} dy^0 \int d^3x d^3y \nabla_x \cdot \mathbf{j}_F^a(x) D_0(x-y) \nabla_y \cdot \mathbf{j}_F^a(y)} \Big|_{t \rightarrow i\tau} \quad (53)$$

where the fermion current is

$$\mathbf{j}_F^a(x) = -i\psi^\dagger(x)(\boldsymbol{\sigma}\tau^a)\psi(x) \quad (54)$$

and $D_0(x-y)$ denotes the free pion propagator, which in momentum space and in the euclidean world reads

$$\tilde{D}_0(q, \omega_n) = \frac{1}{\omega_n^2 + q^2 + m_\pi^2} \quad (55)$$

with ω_n given of course by (31), this time with n even integer only. We can then follow all our machinery to derive the average value of the interaction term, which looks exactly as before if we disregard its frequency (or time) dependence.

Now from (27) we observe that the diagrams we need to evaluate contain one pion propagator (hence a line with the extrema put at different times) closed by a two-particle Green's function whose time evolution is governed by the trial hamiltonian. Let us now take the limit $\Delta \rightarrow 0$, $\beta \rightarrow \infty$ ($\alpha \rightarrow 0$) as in sec. 6. We recall that the rules for obtaining the FHNC diagrams derived there are not influenced by a possible time dependence in the interaction lines. More explicitly, it is irrelevant if the potential lines in figs. 5 and 6 are

instantaneous or not. In both cases, for a given Feynman diagram, others exist (including, perhaps, equivalent diagrams) such that when these are added together the θ -functions sum up to 1, and all time dependence drops out. Consequently the two-particle Green's function evaluated in the frame of FHNC turns out to be time-independent. Let this be, say, $G_{II}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4)$. The integral we are interested in is then

$$\begin{aligned} & \frac{1}{\beta} \text{Tr} \int d^3x d^3y \int_{-\beta/2}^{\beta/2} dx_0 \int_{-\beta/2}^{\beta/2} dy_0 \\ & D_E(x-y) (-i\boldsymbol{\sigma} \cdot \nabla_x \vec{\tau}) (-i\boldsymbol{\sigma} \cdot \nabla_y \vec{\tau}) G_{II}(\mathbf{x}, \mathbf{y}, \mathbf{x}, \mathbf{y}) . \end{aligned} \quad (56)$$

Now we carry out the integrations over the imaginary times. Using eq. (55), it is a simple matter to show that

$$\begin{aligned} & \frac{1}{\beta} \int_{-\beta/2}^{\beta/2} dx_0 \int_{-\beta/2}^{\beta/2} dy_0 D_E(x-y) \\ &= \frac{1}{\beta} \int_{-\beta/2}^{\beta/2} dx_0 \int_{-\beta/2}^{\beta/2} dy_0 \int \frac{d^3q}{(2\pi)^3} e^{-i\mathbf{q} \cdot (\mathbf{x}-\mathbf{y})} \sum_{n \text{ even}} \frac{e^{i\omega_n(x^0-y^0)}}{\omega_n^2 + \mathbf{q}^2 + m_\pi^2} \\ &= \int \frac{d^3q}{(2\pi)^3} e^{-i\mathbf{q} \cdot (\mathbf{x}-\mathbf{y})} \frac{1}{\mathbf{q}^2 + m_\pi^2} = \frac{e^{-m_\pi|\mathbf{x}-\mathbf{y}|}}{4\pi|\mathbf{x}-\mathbf{y}|} . \end{aligned} \quad (57)$$

The conclusion is that what we need for the calculation is to take the effective potential at zero energy and then to perform the standard FHNC calculations. In the present model, the effective potential is just the OPEP, as one might have expected.

To go beyond this variational approximation, now, we have several possibilities. We can try to improve the variational result by allowing the trial hamiltonian to have a spin-dependent interaction and/or a time dependence by taking $\Delta \neq 0$. Otherwise, we can keep the simpler trial hamiltonian used here, which allows the use of the full FHNC machinery, and we can calculate corrections to the variational result through perturbation theory as described in sec. 2. Implementation of these improvements is currently underway.

IX. CONCLUSIONS AND OUTLOOK

Let us now briefly summarize the results obtained in this paper and discuss the possible developments they naturally suggest.

The central idea in this paper is that of formulating a variational approach for dealing with strongly interacting systems which goes beyond the limitations of the Fermi Hypernetted Chain and Correlated Basis Function methods. This led us to use a path integral approach, where the variational method consists in choosing a trial hamiltonian instead of choosing an ansatz for a nonrelativistic wave function. We have obtained several important results. First, one can define the path integral and choose the trial hamiltonian in such a way that for particular systems for which a nonrelativistic wave function makes sense, our approach produces exactly the same results as the successful FHNC formulation. Second, in this path integral formalism one is not linked to a true hamiltonian, but an effective hamiltonian can be used as well. Thus ultimately we can generalize the FHNC variational techniques for use in studying the enormous variety of strongly correlated systems for which the usual FHNC cannot be directly applied because a formulation in terms of nonrelativistic wave functions breaks down. Thirdly, we have shown how corrections to a static variational approximation can be added by choosing a more general trial hamiltonian so to improve the variational energy and by including perturbative corrections in the difference between the true and trial hamiltonians within a compact path integral formulation.

Having first briefly described the variational principle in the Feynman path integral formulation, we proceeded to define our approach by using the FHNC and CBF approaches as motivation. Since these latter approaches treat correlations between particles as more important than independent particle kinetic energies, in our approach the fundamental simplification with respect to the true hamiltonian h we chose for our trial hamiltonian h_0 was to modify its one-body piece. For much of the paper we limited ourselves to the case of a time-independent h_0 , and throughout we only considered spin-independent interactions in h_0 . We made a specific simple choice of the one-body term in h_0 which depends on a parameter $\alpha = \beta\Delta$, and we have shown that in the particular case $\alpha \rightarrow 0$ our expansion scheme in terms of Feynman diagrams exactly reproduces the FHNC results for a variational wave function of the Jastrow type. We also showed that in the limit $\alpha \rightarrow \infty$, the time integrals are also simple, if not as trivial as in the case $\alpha = 0$. We showed that this other limit

corresponds to a new approximation scheme which has the same diagrammatic structure as the FHNC except with different coefficients in front of each diagram.

Finally, to show how our method works in practice, we have shown that the variational scheme can be applied to a quantum-field-theoretical case, a system of interacting nucleons and pions. We have proved a minimal but highly nontrivial result — namely, that in a system containing dynamical pions a variational procedure built up upon the static one pion exchange potential still provides an upper bound to the energy.

The present paper was mostly devoted to proving the correctness of the method and its equivalence, in a very particular case, with the available FHNC calculations. However, it opens several interesting perspectives which we want to discuss now. First, we limited ourselves to trial hamiltonians which correspond to the Jastrow ansatz for the wave function in the usual FHNC approach. State-dependent interactions in h_0 can be handled on the same footing as those described here. Very likely, as some preliminary results seem to indicate, the method presented here could provide a very useful tool to overcome the limitations of the Single Operator Chain approximation.

Next, we have to exploit the new possibilities offered by the present approach. First, energy-dependent correlations can be accounted for, thus improving upon the usual calculations carried out with phenomenological nuclear potentials. Second, an extension to relativistic systems is now allowed, potentially cumbersome but in principle feasible. In fact, again we are faced, in a relativistic system, with a case where a trial wave function loses its sense but our (eventually time-dependent) trial hamiltonian does not. Third, in connection with the previous point, the possibility of carrying out a variational calculation with the Bonn potential¹⁵ is now offered. Note that using energy-dependent interactions in the trial hamiltonian (energy-dependent correlations in the FHNC language) allows for an improvement upon the results of sec. 8, going beyond the static limit of the potential.

Finally, another promising application of our approach is to quantum field theory, as indeed we briefly demonstrated in sec. 8. Variational methods have been little used in field theory up to now (see, for example,¹⁶⁻¹⁸), and to our knowledge nothing of the sort

introduced here to deal with strongly correlated systems has been explored in the field theoretical problems. Our approach thus opens up new possibilities in this direction. The obvious, if ambitious, application would be to study low energy bound states of quantum chromodynamics, where the usual perturbative methods are hopeless. There are two paths one can follow in this respect. One is to study euclidean path integrals as in sec. 8, obtaining an effective lagrangian through functional integration. A second possibility, which might overcome some of the problems mentioned by Feynman¹⁹, is first to develop an effective hamiltonian using Wilsonian renormalization group methods — a promising approach in this direction is proposed and detailed in²⁰ — and then to analyze this effective, frequency-dependent hamiltonian with our path integral variational methods. Indeed, it was the availability of powerful hamiltonian methods such as the variational principle which helped lead Wilson to develop his renormalization group approach²¹. In either of the approaches to field theoretical systems mentioned here, of course, one has difficult renormalization problems to overcome.

It is our hope, then, that the variational approach described here will eventually provide an important tool for studying many different types of strongly correlated systems for which the usual perturbative techniques are insufficient, and that only a small number of the potential applications of our approach have been mentioned here.

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APPENDIX A: DERIVATION OF EQ. (8)

We show here that the first and third terms on the r.h.s. of eq. (7) cancel even for a time-dependent potential $h(\tau)$.

Let us define a suitable “partition function”

$$Z_0^\lambda = \int D[\psi^\dagger \psi] e^{-\lambda \int_{-\beta/2}^{\beta/2} h_0(\tau) d\tau}, \quad (\text{A1})$$

so that

$$-\frac{\partial}{\partial \lambda} \log Z_0^\lambda = \frac{\int D[\psi^\dagger \psi] \left(\int_{-\beta/2}^{\beta/2} h_0(\tau) d\tau \right) e^{-\lambda \int_{-\beta/2}^{\beta/2} h_0(\tau) d\tau}}{\int D[\psi^\dagger \psi] e^{-\lambda \int_{-\beta/2}^{\beta/2} h_0(\tau) d\tau}}. \quad (\text{A2})$$

By comparison with (3)

$$\left\langle \int_{-\beta/2}^{\beta/2} h_0(\tau) d\tau \right\rangle_{h_0} = -\frac{\partial}{\partial \lambda} \log Z_0^\lambda \Big|_{\lambda=1}. \quad (\text{A3})$$

Now we represent $h_0(\tau)$ in (A2) as the Fourier series $\sum_{\omega_n} e^{i\omega_n \tau} \tilde{h}_0(\omega_n)$ with $\omega_n = \pi n/\beta$, so that as $\beta \rightarrow \infty$

$$\int_{-\beta/2}^{\beta/2} h_0(\tau) d\tau \longrightarrow \beta \tilde{h}_0(0). \quad (\text{A4})$$

In this limit, then, the path integral is equivalent to a trace over the eigenstates of $\tilde{h}_0(0)$, whose eigenvalues we write as $\tilde{\epsilon}_n$. Thus

$$\begin{aligned} -\frac{1}{\beta} \frac{\partial}{\partial \lambda} \log Z_0^\lambda &\longrightarrow \frac{\int D[\psi^\dagger \psi] \tilde{h}_0(0) e^{-\lambda \beta \tilde{h}_0(0)}}{\int D[\psi^\dagger \psi] e^{-\lambda \beta \tilde{h}_0(0)}} \\ &\longrightarrow \frac{\sum_n \tilde{\epsilon}_n e^{-\lambda \beta \tilde{\epsilon}_n}}{\sum_n e^{-\lambda \beta \tilde{\epsilon}_n}}. \end{aligned} \quad (\text{A5})$$

As $\beta \rightarrow \infty$, of course, the lowest energy state dominates this average, giving the result

$$-\lim_{\beta \rightarrow \infty} \frac{1}{\beta} \frac{\partial}{\partial \lambda} \log Z_0^\lambda = \tilde{\epsilon}_0,$$

which does not depend upon λ . This implies

$$\lim_{\beta \rightarrow \infty} \frac{1}{\beta} \frac{\partial}{\partial \lambda} \log Z_0^\lambda = \int_0^1 d\lambda \lim_{\beta \rightarrow \infty} \frac{1}{\beta} \frac{\partial}{\partial \lambda} \log Z_0^\lambda = \lim_{\beta \rightarrow \infty} \frac{1}{\beta} \log Z_0^\lambda \Big|_{\lambda=1} \quad (\text{A6})$$

since Z is normalized such that $\log Z_0^\lambda \Big|_{\lambda=0} = 0$. Comparing (3), (A3) and (A6), we end up with

$$E_0 \leq \lim_{\beta \rightarrow \infty} \frac{1}{\beta} \left\langle \int_{-\beta/2}^{\beta/2} h d\tau \right\rangle_{h_0}. \quad (\text{A7})$$

APPENDIX B: BOUNDARY CONDITIONS ON THE PATH INTEGRAL

Here we show explicitly the two choices of boundary conditions on the ferm-ionic euclidean path integral discussed in Sec. 4. Further details may be found, for example, in Ref.¹³.

The standard notation

$$Z = \int D[\psi^\dagger, \psi] e^{-\int_{-\beta/2}^{\beta/2} h_0[\psi^\dagger, \psi] d\tau} \quad (\text{B1})$$

used in the text is a misleading shorthand for

$$Z(z_f^*, z_i) = \int_{z(-\beta/2)=z_i}^{z^*(\beta/2)=z_f^*} \lim_{N \rightarrow \infty} \prod_{n=-N}^N d\mu[z(\beta n/2N)] e^{-\int_{-\beta/2}^{\beta/2} h_0(z, z^*) d\tau}, \quad (\text{B2})$$

where the integration measure is

$$d\mu[z] = \prod_q dz_q^* dz_q e^{-z_q^* z_q}. \quad (\text{B3})$$

Here h_0 is assumed time-independent for simplicity, and the classical Grassman variables z and z^* correspond to the nonorthogonal coherent states

$$|z\rangle = e^{\sum_q z_q a_q^\dagger} |0\rangle \quad \text{and} \quad \langle z| = \langle 0| e^{\sum_q z_q^* a_q}, \quad (\text{B4})$$

with $|0\rangle$ the Fock vacuum. These coherent states are nonorthogonal superpositions of Fock states with differing numbers of particles, and their overlap is

$$\langle z|z'\rangle = e^{\sum_q z_q^* z'_q} \equiv e^{z^* z'}. \quad (\text{B5})$$

The variables z_i and z_f^* are not integrated over in (B2), which is equivalent to the matrix element

$$\langle z_f| e^{-\beta h_0} |z_i\rangle. \quad (\text{B6})$$

The usual choice of boundary conditions is to set $z_f^* = -z_i^*$ and to integrate over z_i

$$Z = \int d\mu(z_i) Z(-z_i^*, z_i), \quad (\text{B7})$$

so that the generating function Z becomes a trace over all Fock states — that is, the partition function. Then the $\beta \rightarrow \infty$ limit will pick out the ground state, provided h_0 has a unique ground state. If this is not the case, as for the FHNC choice $\Delta = 0$, we must work a little harder to ensure that (B2) is equivalent to the desired matrix element. We can use the closure relation

$$\int d\mu[z] |z\rangle \langle z| = 1 \quad (\text{B8})$$

to represent any state $|\phi\rangle$ as

$$|\phi\rangle = \int d\mu[z] |z\rangle \langle z|\phi\rangle . \quad (\text{B9})$$

Thus in the $\Delta = 0$ case we must take our shorthand expression (B1) to represent

$$Z = \int d\mu[z_f] d\mu[z_i] \langle \phi_0 | z_f \rangle Z(z_f^*, z_i) \langle z_i | \phi_0 \rangle \quad (\text{B10})$$

in order to ensure that we are evaluating the matrix element $\langle \phi_0 | e^{-\beta h_0} | \phi_0 \rangle$. Here $|\phi_0\rangle$ is the free Fermi gas ground state as in Sec. 4, so that

$$\langle \phi_0 | z \rangle = \prod_{q \leq k_F} z_q. \quad (\text{B11})$$

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FIGURES

FIG. 1. Third order Feynman diagram

FIG. 2. Fourth order Feynman diagram

FIG. 3. Time-ordered “Goldstone” diagrams corresponding to fig. 2

FIG. 4. Example of separation of propagators into two terms

FIG. 5. Two subdiagrams which sum to give a time-independent diagrammatic structure

FIG. 6. A further example of summation to form time-independent diagrams

FIG. 7. Summation of ladder diagrams